Supersymmetry and the Hartmann Potential of Theoretical Chemistry *

GARDO GARNET BLADO †

Division of Science and Mathematics University of Minnesota, Morris

Morris, MN, U.S.A. 56267-2128

Abstract

The ring-shaped Hartmann potential $V = \eta\sigma^2\epsilon_0\left(\frac{2a_0}{r} - \frac{\eta a_0^2}{r^2 sin^2\theta}\right)$ was introduced in quantum chemistry to describe ring-shaped molecules like benzene. In this article, the supersymmetric features of the Hartmann potential are discussed. We first review the results of a previous paper in which we rederived the eigenvalues and radial eigenfunctions of the Hartmann potential using a formulation of one-dimensional supersymmetric quantum mechanics (SUSYQM) on the half-line $[0, \infty)$. A reformulation of SUSYQM in the full line $(-\infty, \infty)$ is subsequently developed. It is found that the second formulation makes a connection between states having the same quantum number L but different values of $\eta\sigma^2$ and quantum number N. This is in contrast to the first formulation, which relates states with identical values of the quantum number N and $\eta\sigma^2$ but different values of the quantum number L.

Key words: supersymmetry, Hartmann potential, supersymmetric quantum mechanics, ring-shaped potential, superpotential

*to be published at the *Theoretica Chimica Acta*

†e-mail: bladogg@cda.mrs.umn.edu; FAX: (612) 589-6371

1 Introduction

In 1972, an exactly solvable ring-shaped potential was introduced by H. Hartmann [1]. The Hartmann potential is given by the following expression,

$$V = \eta\sigma^2\epsilon_0 \left(\frac{2a_0}{r} - \frac{\eta a_0^2}{r^2 sin^2\theta} \right) \tag{1}$$

where

$$a_0 = \frac{\hbar^2}{\mu e^2} \qquad \text{and} \qquad \epsilon_0 = -\frac{1}{2}\frac{\mu e^4}{\hbar^2} \tag{2}$$

μ is the particle mass, η and σ are positive real parameters which range from about 1 to 10 in theoretical chemistry applications [2] and r, θ are in spherical coordinates. In a previous paper [3], SUSYQM techniques were used to rederive the eigenvalues and eigenfunctions of the Hartmann potential. In this article, we further explore its supersymmetric quantum mechanical features by a second formulation of SUSYQM. This analysis is inspired by the analysis made for the hydrogen atom using supersymmetry (SUSY) in reference [4].

The concept of supersymmetry (SUSY) has been used in particle physics in the past two decades [5, 6]. It was discovered in 1971 by Gel'fand and Likhtman [7]. Simply put, supersymmetry is a symmetry which relates fermionic and bosonic degrees of freedom. At present, particle physicists believe that it is an essential ingredient in unifying the four fundamental forces in nature namely the electromagnetic, weak, strong and gravitational interactions.

Supersymmetric theories of the four fundamental interactions entail the presence of SUSY partners which have the same mass as their corresponding ordinarily observed particles.[1] Unfortunately, these have not been observed in nature. To make sense out of this experimental fact, theorists believe that SUSY must be "broken" at ordinary energies. The search for a mechanism to break SUSY led Witten [8] in 1981 to study SUSY breaking in the simplest case of SUSY quantum mechanics. In fact, studies in SUSYQM during its early years, were confined solely for understanding SUSY breaking.

However, it was eventually discovered that SUSYQM can have interesting applications besides its use in the study of SUSY breaking. At present, it has found its way in many areas of physics including atomic physics, statistical physics, nuclear physics. etc. [9] and most recently in quantum chemistry [3]. Through the present article, the author hopes to contribute towards the further utilization of SUSYQM in theoretical chemistry.

[1]For example, the SUSY partner of the electron is called a selectron while that of a photon is a photino.

In section 2, a pedagogical introduction to SUSYQM is developed. Only the concepts and equations which are essential for the present paper are presented.

We present the the SUSYQM features of the Hartmann potential in section 3. In subsection 3.1, we review our results from reference [3] [2] where we formulated SUSYQM in the half-line $[0, \infty)$. Subsection 3.2 discusses the second formulation of SUSYQM in the full-line $(-\infty, \infty)$. Subsequently, this formulation is compared with the first formulation of subsection 3.1.

We give some conclusions in section 4.

[2] We do this for completeness and to facilitate the comparison with the second formulation.

2 Supersymmetric Quantum Mechanics [3]

As mentioned in the Introduction, SUSY was first applied to particle physics, whose language is quantum field theory. In quantum field theory, a particle is represented by a component field φ_i and its dynamics is described by a lagrangian density $\mathcal{L}(\varphi_i, \partial_\mu \varphi_i)$ where $\left[\partial_\mu \equiv \left(\frac{1}{c}\frac{\partial}{\partial t}, \vec{\nabla}\right)\right]$. The word "supersymmetry" was originally used to describe the symmetry which transforms a field φ to another field ψ whose intrinsic spin differs from φ by $\frac{1}{2}\hbar$. In SUSYQM, which will be described here, we will use the term "supersymmetry" in a more general sense. It will be used to denote systems which can be described by the SUSY algebra.

SUSYQM [8, 10] is characterized by the existence of the charge operators Q_i, where $i = 1, 2, \ldots, N$ such that they obey the SUSY algebra (denoted by sqm(N)),

$$\{Q_i, Q_j\} = \delta_{ij} H_{ss} \qquad [Q_i, H_{ss}] = 0 \tag{3}$$

where H_{ss} is the supersymmetric Hamiltonian, { } and [ ] are anticommutator and commutator respectively. We consider only sqm(2) with charge operators Q_1 and Q_2 and construct the linear combinations

$$Q = \frac{1}{\sqrt{2}}\left(Q_1 + iQ_2\right) \qquad \text{and} \qquad Q^\dagger = \frac{1}{\sqrt{2}}\left(Q_1 - iQ_2\right) \ . \tag{4}$$

From equations 3 and 4, The SUSY algebra is then

$$\left\{Q, Q^\dagger\right\} = H_{ss}, \qquad Q^2 = 0, \qquad \left(Q^\dagger\right)^2 = 0 \tag{5}$$

with

$$[Q, H_{ss}] = 0 \qquad \text{and} \qquad \left[Q^\dagger, H_{ss}\right] = 0. \tag{6}$$

The above SUSY algebra can be realized by letting

$$Q = \begin{bmatrix} 0 & 0 \\ A^- & 0 \end{bmatrix} \ ; \ Q^\dagger = \begin{bmatrix} 0 & A^+ \\ 0 & 0 \end{bmatrix} \tag{7}$$

where

$$\left(A^-\right)^\dagger = A^+. \tag{8}$$

From equations 5 and 7, the supersymmetric hamiltonian is

$$H_{ss} = \begin{bmatrix} H_1 & 0 \\ 0 & H_2 \end{bmatrix} \tag{9}$$

where

$$H_1 = A^+A^- \qquad \text{and} \qquad H_2 = A^-A^+. \tag{10}$$

The hamiltonians H_1 and H_2 are said to be "supersymmetric" partners of each other. H_1 is called the "Bose" sector while H_2 is the "Fermi" sector.

The hamiltonian of the Schrödinger equation can always be factorized in the form of equation 10. Consider the hamiltonian [9]

$$H_1 = -\frac{1}{2}\frac{d^2}{dx^2} + V_1(x) \tag{11}$$

such that

$$H_1\psi^n_{(1)} = \left[-\frac{1}{2}\frac{d^2}{dx^2} + V_1(x)\right]\psi^n_{(1)} = E^n_{(1)}\psi^n_{(1)} \tag{12}$$

where $V_1(x)$ is chosen such that the ground state $\psi^0_{(1)}$ has an energy eigenvalue equal to zero. The hamiltonian in equation 11 can be put in the form of equation 10 by letting

$$A_1^- = \frac{1}{\sqrt{2}}\left(\frac{d}{dx} + W_1\right) \qquad \text{and} \qquad A_1^+ = \frac{1}{\sqrt{2}}\left(-\frac{d}{dx} + W_1\right) \tag{13}$$

provided that the "superpotential" W_1 satisfies the Ricatti equation

$$V_1(x) = \frac{1}{2}\left[W_1^2 - \frac{dW_1}{dx}\right] . \tag{14}$$

As long as equation 14 has a solution W_1, the one-dimensional Schrödinger equation can be made supersymmetric by the construction given in equations 13, 10 and 9. The challenge then in using SUSYQM techniques is not in the mechanics of the construction of just any SUSY hamiltonian, but in finding a suitable superpotential (or $V_1(x)$) to construct a SUSY hamiltonian which will be relevant to the problem at hand. It is a common practice to choose or pose as an ansatz the W_1 to solve a physical problem [11, 12].

The SUSY partner of H_1, namely H_2 is then given by

$$H_2 = -\frac{1}{2}\frac{d^2}{dx^2} + V_2(x) = A_1^-A_1^+ \tag{15}$$

where

$$V_2(x) = \frac{1}{2}\left[W_1^2 + \frac{dW_1}{dx}\right] . \tag{16}$$

Note that H_2 is altogether a new hamiltonian. An astute reader will immediately realize that one can repeat the procedure in constructing H_2 from H_1 to construct an H_3 from H_2 such that

$$H_2 = A_2^+A_2^- \tag{17}$$

with

$$A_2^- = \frac{1}{\sqrt{2}}\left(\frac{d}{dx} + W_2\right) \qquad \text{and} \qquad A_2^+ = \frac{1}{\sqrt{2}}\left(-\frac{d}{dx} + W_2\right) \tag{18}$$

and with a new Ricatti equation

$$V_2(x) = \frac{1}{2}\left[W_2^2 - \frac{dW_2}{dx}\right]. \tag{19}$$

W_2 in equation 19 is then solved to construct $A_2^{\pm}$. H_3 can then be constructed as

$$H_3 = -\frac{1}{2}\frac{d^2}{dx^2} + V_3(x) = A_2^- A_2^+ \tag{20}$$

where

$$V_3(x) = \frac{1}{2}\left[W_2^2 + \frac{dW_2}{dx}\right] . \tag{21}$$

We can evidently construct a "hierarchy" of SUSY-partner hamiltonians H_1, H_2, H_3, ..., H_n starting from H_1.

Let us go back to the first two hamiltonians we started with namely H_1 and H_2. Since $V_1(x)$ in equation 11 is chosen such that its ground state wave function $\psi_{(1)}^0$ has eigenvalue equal to zero, equation 10 gives

$$H_1\psi_{(1)}^0 = 0 \quad \Longrightarrow \quad A_1^+ A_1^- \psi_{(1)}^0 = 0. \tag{22}$$

Equation 22 implies

$$A_1^-\psi_{(1)}^0 = 0. \tag{23}$$

With equation 13 and knowing W_1, equation 23 allows one to calculate the ground state of H_1 by solving the resulting first order differential equation.

Consider any eigenstate of H_1, $\psi_{(1)}^n$ with energy $E_{(1)}^n$. We have

$$H_1\psi_{(1)}^n = E_{(1)}^n\psi_{(1)}^n \tag{24}$$

or from equation 10

$$A_1^+ A_1^- \psi_{(1)}^n = E_{(1)}^n\psi_{(1)}^n. \tag{25}$$

Applying A_1^- to equation 25, $A_1^- A_1^+ \left(A_1^-\psi_{(1)}^n\right) = E_{(1)}^n A_1^-\psi_{(1)}^n$ or with equation 15

$$H_2\left(A_1^-\psi_{(1)}^n\right) = E_{(1)}^n\left(A_1^-\psi_{(1)}^n\right). \tag{26}$$

Conversely, consider an eigenfunction $\psi_{(2)}^n$ of H_2 with eigenvalue $E_{(2)}^n$. With equation 15, we get $H_2\psi_{(2)}^n = A_1^- A_1^+\psi_{(2)}^n = E_{(2)}^n\psi_{(2)}^n$. Multiplying by A_1^+, we have, $A_1^+ A_1^-\left(A_1^+\psi_{(2)}^n\right) = E_{(2)}^n A_1^+\psi_{(2)}^n$. With equation 10

$$H_1\left(A_1^+\psi_{(2)}^n\right) = E_{(2)}^n\left(A_1^+\psi_{(2)}^n\right). \tag{27}$$

Equations 26 and 27 imply that the hamiltonians H_1 and H_2 have identical eigenvalues except for the ground state $\psi^0_{(1)}$ of H_1 (since $A_1^- \psi^0_{(1)} = 0$ in equation 26 and this is unnormalizable). In addition, we can see that if you know an eigenfunction of H_1, i.e. $\psi^n_{(1)}$, then an eigenfunction $A_1^- \psi^n_{(1)}$ of H_2 can be formed. Similarly, an eigenfunction $A_1^+ \psi^n_{(2)}$ of H_1 can be formed given an eigenfunction $\psi^n_{(2)}$ of H_2. The preceding analysis can then be extended to the hierarchy of hamiltonians discussed earlier. These observations are illustrated in figure 1.

Herein lies a very important consequence of SUSYQM. The energy eigenfunctions of the hierarchy of hamiltonians are related by the SUSY operators $A^{\pm}$. If one knows the eigenvalues and eigenfunctions of a particular H_n, then one can get the eigenvalues and eigenfunctions of its SUSY partner.

Note that what we have discussed is SUSYQM in one dimension.There had been work done in doing SUSYQM in two or more dimensions [13, 14]. To be able to apply one dimensional SUSYQM to the Hartmann potential, we will do a separation of variables of the resulting Schrödinger equation. In forming a hamiltonian from a separated one dimensional differential equation that can be an element of an H_{ss}, this one dimensional differential equation must be of the form of equation 12 (no first derivative term) and must yield an infinite tower of states as for H_n of figure 1 [15]. As we will see, upon separation of variables for the Hartmann potential, only the radial equation yields an interesting SUSY.

3 Supersymmetry in the Hartmann Hamiltonian

With the SUSYQM concepts introduced in section 2, we are now ready to discuss the SUSY features of the radial equation of the Schrödinger equation of the Hartmann potential in spherical coordinates.

3.1 Calculation of the eigenvalues and radial eigenfunctions

The Schrödinger equation in spherical coordinates for a particle of mass μ subjected to the Hartmann potential in equation 1 is given by

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi + \left[\frac{2\eta\sigma^2\epsilon_0 a_0}{r} - \frac{\eta^2\sigma^2 a_0^2\epsilon_0}{r^2 sin^2\theta}\right]\psi = E\psi \ . \tag{28}$$

Assuming a solution

$$\psi = R(r)\Theta(\theta)\Phi(\phi) \tag{29}$$

equation 28 can be separated into three differential equations [1]

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2 \tag{30}$$

$$\frac{1}{sin\theta}\frac{d}{d\theta}\left(sin\theta\frac{d\Theta}{d\theta}\right) - \left(\frac{M^2}{sin^2\theta} - L(L+1)\right)\Theta = 0 \tag{31}$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - L(L+1)\frac{R}{r^2} + \frac{8\pi^2\mu}{h^2}\left(E + \frac{\eta\sigma^2 e^2}{r}\right)R = 0 \tag{32}$$

where

$$M^2 = m^2 + \eta^2\sigma^2 \ . \tag{33}$$

Looking at equations 30 to 32, we realize that these closely resemble the separated equations of the hydrogen atom [16]. As shown by reference [15], the only interesting separable SUSY in the hydrogen atom in spherical coordinates results from the radial equation. Their argument is as follows. Looking at equation 30, and comparing it with equation 12, we see that $V_1 = 0$. Equation 31 on the other hand can be cast to a form similar to equation 12 by multiplying it by a modulation factor $\frac{f(cos\theta)}{[1-cos^2\theta]^{1/2}}$. The eigenvalue of $f(cos\theta)$ is zero and no infinite tower of states can be generated. Hence, the Φ and Θ solutions cannot be given by SUSYQM. They can be solved by conventional means [1]

$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}}e^{im\phi}, \qquad m = 0,\ \pm1,\ \pm2, \ldots \tag{34}$$

$$\Theta(\theta) \sim \mathcal{P}_L^{|M|}(cos\theta), \qquad L = \nu' + |M|\,, \qquad \nu' = 0,\ 1,\ 2, \ldots \tag{35}$$

where $\mathcal{P}_L^{|M|}(cos\theta)$ are the associated Legendre polynomials.

The radial equation 32 can be cast into a form similar to 12 by letting

$$R = \frac{u}{r}\ . \tag{36}$$

Substituting equation 36 into equation 32, yields

$$H_L u = \left[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{L(L+1)}{2r^2} - \frac{\gamma}{r}\right] u = \frac{\mu E}{\hbar^2} u \tag{37}$$

with

$$\gamma \equiv \frac{\mu\eta\sigma^2 e^2}{\hbar^2}. \tag{38}$$

Equation 37 is similar to that of the hydrogen atom's radial equation. We thus claim that we can obtain the eigenvalues and radial eigenfunctions by looking at the hamiltonian [11]

$$\mathcal{H}_L = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{L(L+1)}{2r^2} - \frac{\gamma}{r} + \frac{1}{2}\left(\frac{\gamma}{L+1}\right)^2 \tag{39}$$

which yields a Ricatti equation (from equations 39, 11 and 14)

$$\frac{L(L+1)}{2r^2} - \frac{\gamma}{r} + \frac{1}{2}\left(\frac{\gamma}{L+1}\right)^2 = \frac{1}{2}\left[W_L^2 - \frac{dW_L}{dr}\right] \tag{40}$$

whose solution is

$$W_L = -\frac{L+1}{r} + \frac{\gamma}{L+1}\ . \tag{41}$$

Equation 41 and 13 yield

$$A_L^{\pm} = \frac{1}{\sqrt{2}}\left(\mp\frac{d}{dr} - \frac{L+1}{r} + \frac{\gamma}{L+1}\right). \tag{42}$$

From equation 42 and 15, we construct the SUSY-partner hamiltonian of $\mathcal{H}_L$ in equation 39,

$$\mathcal{H}_{L+1} = A_L^- A_L^+ = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{(L+1)(L+2)}{2r^2} - \frac{\gamma}{r} + \frac{1}{2}\left(\frac{\gamma}{L+1}\right)^2\ . \tag{43}$$

Comparing equations 37 and 39 and with equation 43, we realize that

$$\mathcal{H}_L = H_L + \frac{1}{2}\left(\frac{\gamma}{L+1}\right)^2 \tag{44}$$

$$\mathcal{H}_{L+1} = H_{L+1} + \frac{1}{2}\left(\frac{\gamma}{L+1}\right)^2\ . \tag{45}$$

Let us now start to build up the radial eigenfunctions and in the process get the eigenvalues. Given an $|M|$ value, the lowest L value is $L = |M|$, as can be seen in equation 35. It is apparent from equations 44 and 45 that we can build the states of the hierarchy of hamiltonians as in figure 1. This is illustrated in figure 2.

Since $\mathcal{H}_{|M|}$ ($\mathcal{H}_{|M|+1}$) and $H_{|M|}$ ($H_{|M|+1}$) differ only by a constant, (see equations 44 and 45) every eigenfunction of $\mathcal{H}_{|M|}$ ($\mathcal{H}_{|M|+1}$) will be an eigenfunction of $H_{|M|}$ ($H_{|M|+1}$). Hence, all we have to do is to solve for the eigenfunctions of $\mathcal{H}_L$. The actual energy for H_L can be found by letting H_L act on the eigenfunctions of $\mathcal{H}_L$.

For an arbitrary L, equations 23 and 42 give, for the ground states of $\mathcal{H}_L$, $\psi^0_{(L)}$, the first order differential equation

$$\frac{1}{\sqrt{2}}\left(\frac{d}{dr} - \frac{L+1}{r} + \frac{\gamma}{L+1}\right)\psi^0_{(L)} = 0 \tag{46}$$

which can easily be solved as

$$\psi^0_{(L)} = \mathcal{N}_L\, r^{L+1} exp(-\kappa_L r) \tag{47}$$

where

$$\kappa_L \equiv \frac{\gamma}{L+1}\ . \tag{48}$$

Since L is arbitrary here, we realize that equation 47 is the expression for the eigenfunction for the lowest rung (i.e. the ground state) of the tower of states for each of the hamiltonians in figure 2. Since they are also eigenfunctions of H_L, we can write

$$u_L = \mathcal{N}_L\, r^{L+1} exp(-\kappa_L r) \tag{49}$$

where we illustrate them in figure 3.

To get the actual energy, we let H_L of equation 37 act on equation 49.

$$H_L u_L = \left[-\frac{1}{2}\frac{d^2}{dr^2} + \left(\frac{L(L+1)}{2r^2} - \frac{\gamma}{r}\right)\right] u_L = \frac{\mu E_L}{\hbar^2} u_L\ . \tag{50}$$

After some simplification, this yields

$$E_L = -\frac{\Lambda}{(L+1)^2} \qquad \Lambda = \eta^2\sigma^4\,|\epsilon_0|\,. \tag{51}$$

We characterize the energy by the L quantum number for the moment. From equation 51, we can label the energy levels of figure 3 as in figure 4.

It is apparent from figure 4 that we have to label the solutions u as $u_{|M|+1,\,|M|}$; $u_{|M|+2,\,|M|+1}$; $u_{|M|+3,\,|M|+2}$; ... due to the energy of the states. Knowing the eigenstates

at the lowest rung of the hierarchy of hamiltonians, $u_{|M|+1,\,|M|}$; $u_{|M|+2,\,|M|+1}$; $u_{|M|+3,\,|M|+2}$; etc., we can determine the other states by the action of A_L^+ on these eigenstates as in figure 1. This is illustrated in figure 5.

Note that, for instance, $u_{|M|+3,|M|}$; $u_{|M|+3,|M|+1}$; $u_{|M|+3,|M|+2}$; ... have the same energy $-\frac{\Lambda}{(|M|+3)^2}$, and similarly for other states at the same energy level. It is then evident that given $N \geq |M|+1$, $u_{N,N-1}$; $u_{N,N-2}$; $u_{N,N-3}$; ...; $u_{N,|M|}$ will all have the same energy $-\frac{\Lambda}{N^2}$. Hence, we can say that

$$E_N = -\frac{\Lambda}{N^2}, \qquad \Lambda = \eta^2\sigma^4\left|\epsilon_0\right|, \qquad N = L+1+n', \qquad n' = 0,1,2,\ldots \tag{52}$$

which means that the energy is actually labelled by N and not L. Equation 52 agrees with reference [1].

From figure 5, equations 48, 49, 36 and 42, it can be shown that

$$R_{|M|+1,|M|}(r) = \left[\frac{2\gamma}{|M|+1}\right]^{|M|+3/2}\left[\frac{1}{\Gamma\left(2\left|M\right|+3\right)}\right]^{1/2} r^{|M|}e^{-\gamma r/[|M|+1]} \tag{53}$$

$$R_{|M|+2,|M|+1}(r) = \left[\frac{2\gamma}{|M|+2}\right]^{|M|+5/2}\left[\frac{1}{\Gamma\left(2\left|M\right|+5\right)}\right]^{1/2} r^{|M|+1}e^{-\gamma r/[|M|+2]} \tag{54}$$

$$\begin{aligned} R_{|M|+2,|M|}(r) \;\; = \;\; & -\left[\tfrac{2\gamma}{|M|+2}\right]^{|M|+3/2}\left[\tfrac{1}{2(|M|+2)\Gamma(2|M|+3)}\right]^{1/2} r^{|M|}e^{-\gamma r/[|M|+2]} \\ & \times\left[2\left|M\right|+2-\tfrac{2\gamma r}{|M|+2}\right] \end{aligned} \tag{55}$$

etc. where R_{NL} are normalized by

$$1 = \int_0^\infty \left|R_{NL}\right|^2 r^2 dr \tag{56}$$

and the gamma function properties used are [17]

$$\Gamma(z) = \int_0^\infty e^{-t}t^{z-1}dt; \qquad \Gamma(z+1) = z\Gamma(z)\;. \tag{57}$$

Equations 53, 54 and 55 agree with the normalized R_{NL} of reference [2]. It is obvious that we can eventually get all the expressions of R_{NL}.

To illustrate the procedure more concretely, let us show how we can get $R_{|M|+2,|M|}(r)$. From figure 5,

$$u_{|M|+2,|M|} \sim A^+_{|M|}\; u_{|M|+2,|M|+1}.^3 \tag{58}$$

[3] Note that in equation 3 and in some of the following equations, we use $\sim$ instead of $=$ since the procedure outlined here cannot automatically normalize the eigenfunctions. At the end, we normalize the eigenfunctions using equation 56.

Since $u_{|M|+2,|M|+1}$ is at the lowest rung of $H_{|M|+1}$, we can use equations 48 and 49 which give

$$u_{|M|+2,|M|+1} \sim r^{|M|+2} e^{-\gamma r/[|M|+2]} \,. \tag{59}$$

From equations 42, 3 and 59, we get

$$u_{|M|+2,|M|} \sim \left(-\frac{d}{dr} - \frac{|M|+1}{r} + \frac{\gamma}{|M|+1} \right) r^{|M|+2} e^{-\gamma r/[|M|+2]} \tag{60}$$

which leads to

$$u_{|M|+2,|M|} \sim r e^{-\gamma r/[|M|+2]} \left(-r^{|M|} + \frac{\gamma r^{|M|+1}}{(|M|+2)\,(|M|+1)} \right). \tag{61}$$

Using equations 61 and 36 and rearranging terms, we get

$$R_{|M|+2,|M|} \sim -e^{-\gamma r/[|M|+2]}\; r^{|M|} \left(2 + 2\,|M| - \frac{2\gamma r}{|M|+2} \right) \tag{62}$$

or

$$R_{|M|+2,|M|} = -\mathcal{N} e^{-\gamma r/[|M|+2]}\; r^{|M|} \left(2 + 2\,|M| - \frac{2\gamma r}{|M|+2} \right) \tag{63}$$

where $\mathcal{N}$ is the normalization constant. Normalizing equation 63 using equations 56 and 57 leads to equation 55.

Comparing equations 39 and 43, (discounting the common constant $\frac{1}{2}\left(\frac{\gamma}{L+1}\right)^2$ which just rescales the ground state such that its energy eigenvalue is zero) and with figure 5, we realize that states with quantum numbers (N, L) has for its SUSY partner states with quantum numbers (N, $L+1$).

3.2 Relating eigenstates with different values of $\eta\sigma^2$ and quantum number N

One thing to note about the analysis of subsection 3.1 is that the one dimensional SUSYQM problem was formulated in the half-line [0, ∞) (since $0 \leq r < \infty$). Let us now see the consequences of formulating the SUSYQM problem in the full line $(-\infty, \infty)$ [4].

As a first step, let us rewrite equation 37 by a change of variables given by

$$y \equiv \gamma r = \frac{(\eta\sigma^2)\,\mu e^2}{\hbar^2}\; r \tag{64}$$

with γ given by equation 38. Using equation 64 and the equation for the energy given by equation 52, we can rewrite equation 50 as

$$\left[-\frac{1}{2}\frac{d^2}{dy^2} + \frac{L(L+1)}{2y^2} - \frac{1}{y} \right] u_L = -\frac{1}{2N^2} u_{NL} \,. \tag{65}$$

We now make a second change of variables from y to x such that

$$y = e^x, \quad u_{NL} = e^{x/2}\psi \tag{66}$$

to turn equation 65 into a differential equation in the full line $(-\infty, \infty)$ given by

$$\left[-\frac{1}{2}\frac{d^2}{dx^2} + \frac{e^{2x}}{2N^2} - e^x\right]\psi = -\frac{1}{2}(L+\frac{1}{2})^2\psi \ . \tag{67}$$

It is interesting to note that equation 67 describes a Morse potential $\frac{e^{2x}}{2N^2} - e^x$ with eigenvalues $-\frac{1}{2}(L+\frac{1}{2})^2$. We next find the SUSY-partner hamiltonian of equation 67.

In order to be able to use the results of section 2, we have to chose $V_1(x)$ of equation 67 such that its ground state eigenvalue is zero. Given N, the L values are (from page 11) $N-1$, $N-2$, $N-3$, ..., $|M|$. Hence, the ground state eigenvalue of equation 67 is $-\frac{1}{2}\left(N-1+1/2\right)^2 = -\frac{1}{2}\left(N-1/2\right)^2$. We rewrite equation 67 as

$$H_1\psi = \left[-\frac{1}{2}\frac{d^2}{dx^2} + \frac{e^{2x}}{2N^2} - e^x + \frac{1}{2}\left(N-1/2\right)^2\right]\psi = \left[-\frac{1}{2}(L+1/2)^2 + \frac{1}{2}\left(N-1/2\right)^2\right]\psi \tag{68}$$

with

$$V_1(x) = \frac{e^{2x}}{2N^2} - e^x + \frac{1}{2}\left(N-1/2\right)^2 \tag{69}$$

chosen such that the ground state eigenvalue is zero. We are now ready to get the SUSY-partner hamiltonian of equation 68. From equations 69 and 14, we get the Ricatti equation,

$$\frac{e^{2x}}{2N^2} - e^x + \frac{1}{2}\left(N-1/2\right)^2 = \frac{1}{2}\left[W_1^2 - \frac{dW_1}{dx}\right] \tag{70}$$

whose solution is

$$W_1 = \frac{e^x}{N} + \frac{1}{2} - N \tag{71}$$

From equations 71 and 13, we construct

$$A_1^- = \frac{1}{\sqrt{2}}\left(\frac{d}{dx} + \frac{e^x}{N} + \frac{1}{2} - N\right) \qquad \text{and} \qquad A_1^+ = \frac{1}{\sqrt{2}}\left(-\frac{d}{dx} + \frac{e^x}{N} + \frac{1}{2} - N\right) \ . \tag{72}$$

The SUSY-partner hamiltonian of H_1 in equation 68 is given by equations 72 and 15 yielding

$$H_2 = A_1^- A_1^+ = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{e^{2x}}{2N^2} - \left(1 - \frac{1}{N}\right)e^x + \frac{1}{2}\left(N-1/2\right)^2 \ . \tag{73}$$

From the discussion in section 2, we know that H_2 has the same eigenvalues as H_1 except for the ground state where $L = N-1$ and that the eigenstates $\tilde{\psi}$ of H_2 are related

to that of the eigenstates of H_1 by $\tilde{\psi} \sim A_1^- \psi$. We then write the eigenvalue equation for equation 73 as

$$\begin{aligned} H_2\tilde{\psi} &= \left[-\tfrac{1}{2}\tfrac{d^2}{dx^2} + \tfrac{e^{2x}}{2N^2} - \left(1-\tfrac{1}{N}\right)e^x + \tfrac{1}{2}\left(N-1/2\right)^2\right]\tilde{\psi} \\ &= \left[-\tfrac{1}{2}(L+1/2)^2 + \tfrac{1}{2}\left(N-1/2\right)^2\right]\tilde{\psi}\ . \end{aligned} \tag{74}$$

Summarizing, we have the SUSY-partner eigenvalue equations given by equations 68 and 74 (with the rescaling constant term $\frac{1}{2}\left(N-1/2\right)^2$ cancelled out)

$$\begin{aligned} &\text{a)} \quad \left[-\tfrac{1}{2}\tfrac{d^2}{dx^2} + \tfrac{e^{2x}}{2N^2} - e^x\right]\psi = -\tfrac{1}{2}(L+1/2)^2\psi \\ &\text{b)} \quad \left[-\tfrac{1}{2}\tfrac{d^2}{dx^2} + \tfrac{e^{2x}}{2N^2} - \left(1-\tfrac{1}{N}\right)e^x\right]\tilde{\psi} = -\tfrac{1}{2}(L+1/2)^2\tilde{\psi}\ . \end{aligned} \tag{75}$$

Transforming back to the variable r and the eigenstate u_{NL} using equations 64 and 66, we get from equation 75

$$\begin{aligned} &\text{a)} \quad \left[-\tfrac{1}{2}\tfrac{d^2}{dr^2} - \delta\tfrac{\mu e^2}{\hbar^2}\tfrac{1}{r} + \tfrac{L(L+1)}{2r^2}\right]u_{NL} = -\tfrac{\delta^2}{N^2}\tfrac{\mu^2 e^4}{2\hbar^4}u_{NL} \\ &\text{b)} \quad \left[-\tfrac{1}{2}\tfrac{d^2}{dr^2} - \delta'\tfrac{\mu e^2}{\hbar^2}\tfrac{1}{r} + \tfrac{L(L+1)}{2r^2}\right]\tilde{u}_{N'L} = -\tfrac{\delta'^2}{N'^2}\tfrac{\mu^2 e^4}{2\hbar^4}\tilde{u}_{N'L} \end{aligned} \tag{76}$$

where

$$\begin{aligned} &\text{a)} \quad \delta \equiv \eta\sigma^2 \\ &\text{b)} \quad \delta' = \left(1-\tfrac{1}{N}\right)\delta \\ &\text{c)} \quad N' = N-1 \end{aligned} \tag{77}$$

From equations 76 and 77, it becomes apparent that if we formulate the SUSYQM problem in the full line by the change of variables given by equation 66, states with the quantum numbers (N, L) in a potential with parameter $\eta\sigma^2$ is the SUSY partner of states with quantum numbers ($N-1$, L) but in a potential with parameter $\left(1-\frac{1}{N}\right)\eta\sigma^2$. This relationship is in sharp contrast to that of subsection 3.1 in which states with quantum numbers (N, L) with a potential having parameter $\eta\sigma^2$ has as their SUSY partners, states with quantum numbers (N, $L+1$) with the potential having the same parameter $\eta\sigma^2$. By SUSYQM, we have related states with different $\eta\sigma^2$ and N as SUSY partners in the Hartmann potential.

An illustration of the observations put forth in the preceding paragraph is illustrated in figure 6 for $N = |M|+3$ in which $L = |M|+2,\ |M|+1,\ |M|$. The SUSY-partner states will have $N' = |M|+2$ with $L = |M|+1,\ |M|$. If $\eta\sigma^2$ is the value for the first set of eigenstates, then its SUSY partners will have a value of $\left(1-\frac{1}{N}\right)\eta\sigma^2 = \left(\frac{|M|+2}{|M|+3}\right)\eta\sigma^2$. Note that the actual SUSY eigenvalues are given by $-\frac{1}{2}\left(L+\frac{1}{2}\right)^2$ as in equation 75. In

addition, note carefully that in equation 76, the energy eigenvalues of the SUSY-partner eigenvalue equations are identical since from equation 77

$$\frac{\delta'}{N'} = \frac{\left(1 - \frac{1}{N}\right)\delta}{N-1} = \frac{(N-1)\,\delta/N}{N-1} = \frac{\delta}{N}\,. \tag{78}$$

Hence, in figure 6, the eigenstates have the same energy eigenvalue but different SUSY eigenvalues. We have here a case in which the SUSY partnership does not involve the actual energy eigenvalues.

Another thing to note from figure 6 is that indeed, the spectrum of states of the Fermi sector has all the corresponding states of the Bosonic sector except for its ground state, as expected.

4 Conclusion

In the preceding discussions, we have demonstrated how SUSYQM techniques can be used in the radial equation of the Hartmann potential in theoretical chemistry. By formulating SUSYQM in the half line $[0, \infty)$, we are able to establish a connection between the states with quantum numbers $(N,\ L)$ and $(N,\ L+1)$ and the same parameter values $\eta\sigma^2$. This enabled us to derive the energy eigenvalues and radial eigenfunctions. On the other hand, formulating SUSYQM in the full line $(-\infty, \infty)$, established an interesting SUSY connection between states with quantum numbers $(N,\ L)$ and the parameter value $\eta\sigma^2$ with that of states with quantum numbers $(N-1,\ L)$ and the parameter value $\left(1 - \frac{1}{N}\right)\eta\sigma^2$.

The first formulation basically tells us that SUSYQM techniques can be used as an alternative method of solving the Schrödinger equation. The second formulation reveals the possibility of unraveling new and unexpected relationships between eigenstates with different parameters and quantum numbers.

The key result in SUSYQM is the intimate relationship of the eigenvalues and eigenfunctions of the hierarchy of SUSY-partner hamiltonians. This can be very useful in solving the Schrödinger equation of a complicated hamiltonian if its SUSY-partner hamiltonian is easily solvable.

A very useful result in the present discussion is the fact that $A^-\psi^0 = 0$. This enabled us to solve a first order differential equation (as in equation 46) instead of the second order Schrödinger differential equation to give us the eigenfunctions and eigenvalues of the states at the lowest rung of the tower of states of each of the hamiltonians in the hierarchy. The rest of the eigenfunctions and eigenvalues are then easily computed by applying the corresponding A_L^+ operators to these eigenfunctions.

As already pointed out in this article, the separated equations of the Hartmann potential and the hydrogen atom greatly resemble each other. A number of studies of the SUSY features of the Coulomb problem in hydrogenic atoms have been made over the past years [15, 18, 19]. These studies may very well lead to some further insights into the workings of SUSY in the Hartmann potential due to the similarity of its separated equations with that of the hydrogen atom.

With the above considerations, the author hopes to stimulate further examples of applications of SUSYQM in important problems in theoretical chemistry.

Figure Captions

1. The hierarchy of hamiltonians and the action of the operators $A_n^{\pm}$ on the degenerate eigenstates

2. The energy states of the hierarchy of SUSY-partner hamiltonians from the Hartmann potential

3. The hierarchy of hamiltonians of the Hartmann potential and their ground states. The H_L here are the actual radial hamiltonian for a particular L value.

4. Figure 3 with the energy levels labelled.

5. The energy eigenstates of the Hartmann potential. The action of the A_L^+ operators are explicitly shown to indicate how the other states are obtained from the states at the lowest rung of the hierarchy of hamiltonians.

6. An illustration of SUSY-partner eigenstates identified by (N, L, $\eta\sigma^2$) and ($N-1$, L, $\left(1-\frac{1}{N}\right)\eta\sigma^2$) given $N = |M| + 3$ for the SUSYQM formulation of the Hartmann potential in the full line ($-\infty$,∞). Of course, one can again relate the different eigenstates with the same SUSY eigenvalues by $A_1^{\pm}$ of equation 72.

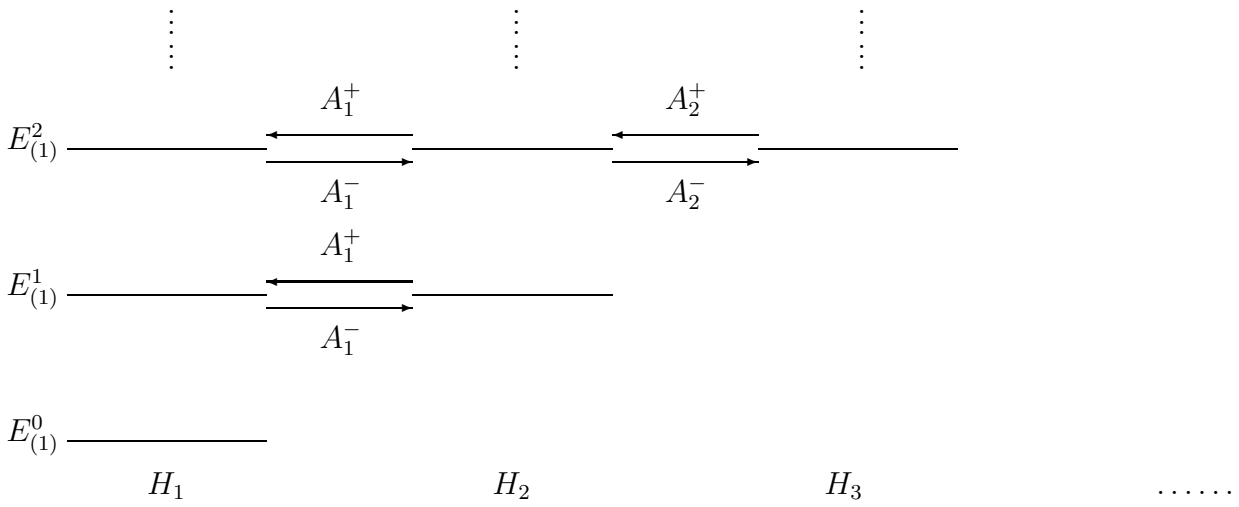

Figure 1: The hierarchy of hamiltonians and the action of the operators $A_n^{\pm}$ on the degenerate eigenstates

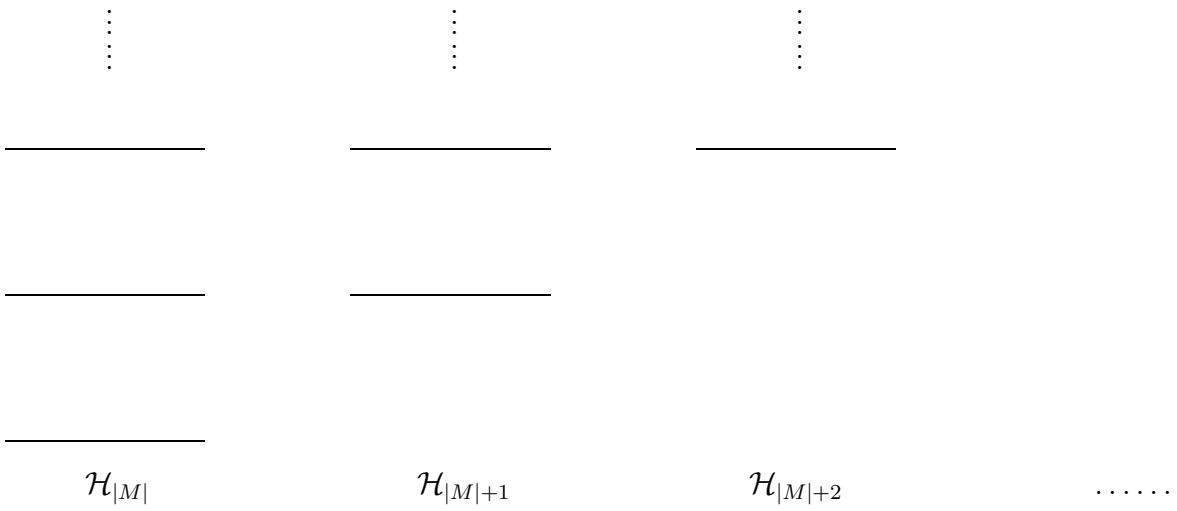

Figure 2: The energy states of the hierarchy of SUSY-partner hamiltonians from the Hartmann potential

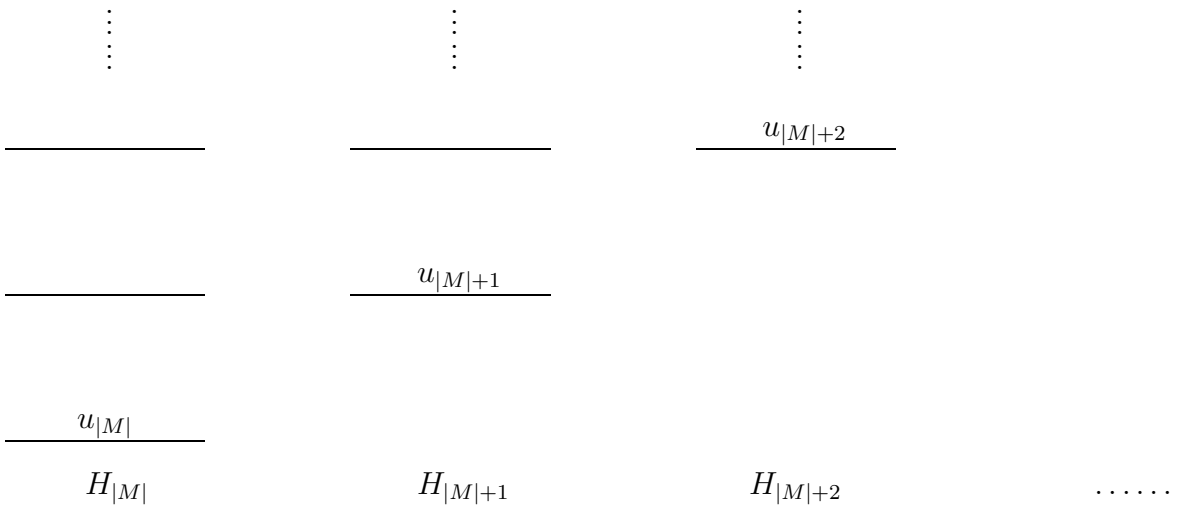

Figure 3: The hierarchy of hamiltonians of the Hartmann potential and their ground states. The H_L here are the actual radial hamiltonian for a particular L value.

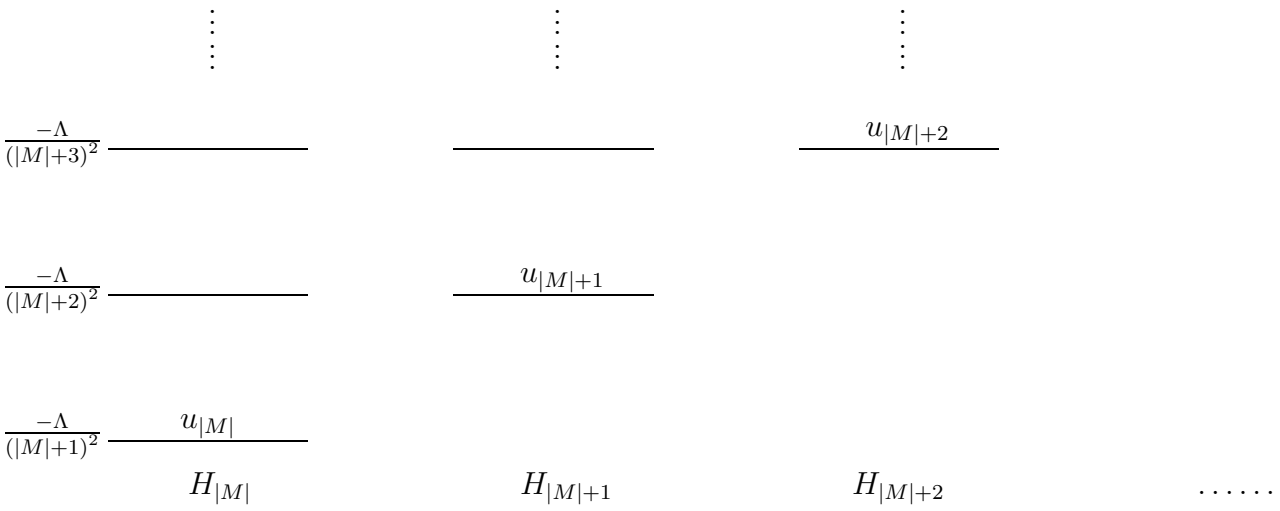

Figure 4: Figure 3 with the energy levels labelled.

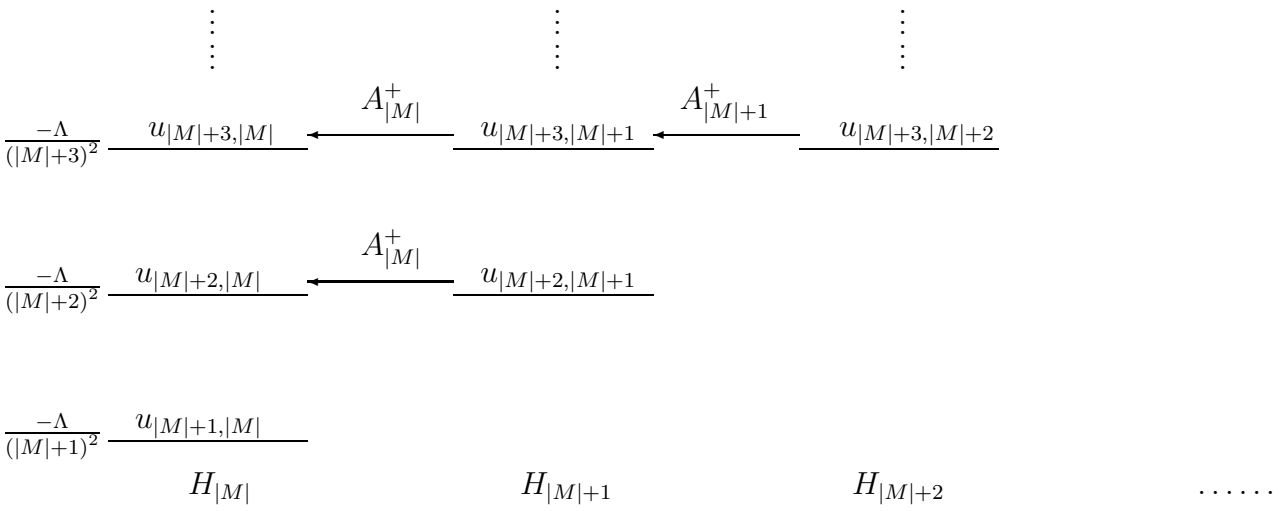

Figure 5: The energy eigenstates of the Hartmann potential. The action of the A_L^+ operators are explicitly shown to indicate how the other states are obtained from the states at the lowest rung of the hierarchy of hamiltonians.

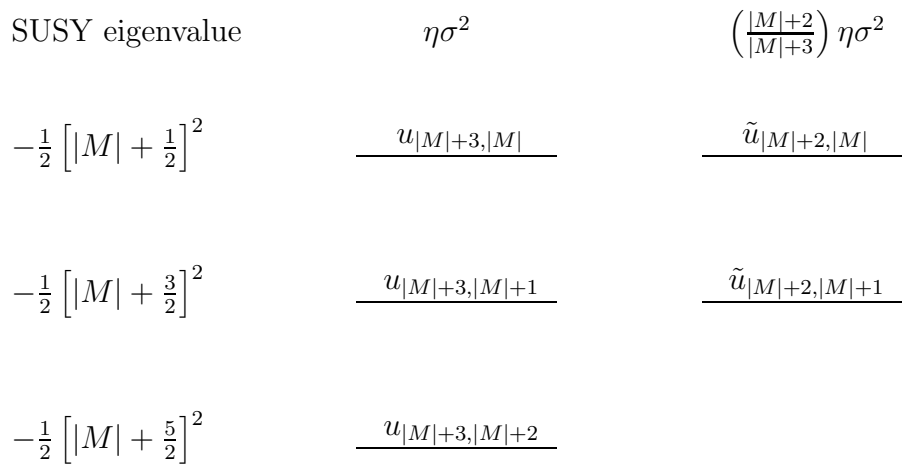

Figure 6: An illustration of SUSY-partner eigenstates identified by $(N,\ L,\ \eta\sigma^2)$ and $\left(N-1,\ L,\ \left(1-\frac{1}{N}\right)\eta\sigma^2\right)$ given $N=|M|+3$ for the SUSYQM formulation of the Hartmann potential in the full line $(-\infty,\infty)$ Of course, one can again relate the different eigenstates with the same SUSY eigenvalues by $A_1^{\pm}$ of equation 72.

References

[1] H. Hartmann, Theor. Chim. Acta **24**, 201 (1972).

[2] H. Hartmann and D. Schuch, Int. J. Quant. Chem. **18**, 125 (1980).

[3] G. G. Blado, Int. J. of Quan. Chem., to be published

[4] R. W. Haymaker and A. R. P. Rau, Am. J. Phys. **54**, 928 (1986).

[5] H. P. Nilles, Phys. Rep. **110**, 1 (1984).

[6] H. E. Haber and G. L. Kane, Phys. Rep. **117**, 75 (1985).

[7] Y. A. Gel'fand and E. P. Likhtman, JETP Lett. **13**, 323 (1971).

[8] E. Witten, Nucl. Phys. **B188**, 513 (1981).

[9] For an exhaustive list of references and review of SUSYQM, see F. Cooper, A. Khare and U. Sukhatme, Phys. Rep. **251**, 267 (1995).

[10] C. V. Sukumar, J. Phys. A: Math. Gen. **18**, 2917 (1985).

[11] F. Schwabl, *Quantum Mechanics* (Springer-Verlag Berlin Heidelberg, 1992).

[12] E. D. Filho and R. M. Ricotta, Mod. Phys. Lett. **A4**, 2283 (1989).

[13] E. D. Filho, Mod. Phys. Lett. **A8**, 63 (1993).

[14] A. A. Andrianov, N. V. Borisov and M. V. Ioffe, Phys. Lett. **A105**, 19 (1984).

[15] R. Bluhm and V. A. Kostelecky, Phys. Rev. **A47**, 794 (1993).

[16] see for example D. J. Griffiths, *Introduction to Quantum Mechanics* (Prentice Hall Inc., 1995).

[17] G. Arfken, *Mathematical Methods for Physicists* (Academic Press Inc., 1970).

[18] V. A. Kostelecky and M. M. Nieto, Phys. Rev. **A32**, 1293 (1985).

[19] V. A. Kostelecky and M. M. Nieto, Phys. Rev. Lett. **53**, 2285 (1984).